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RPPR Final Report
as of 28-Sep-2018

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Proposal Number: 65946MSII **Agreement Number: W911NF-14-1-0559**
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STEM Degrees: 0 **STEM Participants:** 0

Major Goals: NOTE: THIS REPORT WAS SUBMITTED ON BEHALF OF PROFESSOR UPMANYU BY THE PROGRAM MANAGER, BASED ON AN EMAILED DOCUMENT. PROFESSOR UPMANYU COULD NOT OR WOULD NOT ENTER THE REPORT IN THE SYSTEM, SO THE PROGRAM MANAGER FILLED OUT THE FIELDS TO THE BEST OF THEIR ABILITY SO THIS PROJECT COULD BE CLOSED. SOME OF THE DATA MAY BE INACCURATE. THE EMAILED REPORT IS ATTACHED.

1. Explore the variation in segregation profiles as a function of boundary type in Fe-C and Al-Mg systems. Use these variations to extract the strength of the solute-boundary interaction to study the effect of segregation on grain boundary kinetics.

2. Investigate the effect of external stresses on the segregation profile.

3. Investigate the thermodynamic and kinetic mobility of grain boundaries computationally by exploring the equilibrium fluctuations of the segregation interfaces. These values will be used to extract the grain boundary stiffness metric to quantify the drag effect caused by the solute.

Accomplishments: 1. It was found that small amounts of impurities increased instability of a recrystallization front, and these impurities have a strong influence on the kinetics.

2. A combination of theoretical analyses and numerical simulations were performed to study the effect of segregation on equilibrium fluctuations of grain boundaries. The random walk of the dirty interface occurs within a confining solute cloud that itself evolves stochastically in the crystalline matrix, albeit at a much slower rate. The coupled response, a random walk within a random walk, represents a new class of stochastic dynamics. Numerical studies using a combination of Brownian dynamics, kinetic Ising model and all atom simulations of grain boundaries in Fe-C system reveal qualitatively different behavior at multiple time-scale.

3. Employed capillarity fluctuation methods to explore interstitial solute effects on GB stiffness for an asymmetrical tilt grain boundary with different amounts of impurity concentration. Our results showed that solute-loaded grain boundaries exhibit classical rough fluctuation spectrum that allows us to extract their stiffness, and the stiffness increases non-linearly with the solute content. Our study offers a pathway for rational design of stable nanocrystalline alloys.

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Training Opportunities: Nothing to Report

Results Dissemination: Nothing to Report

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

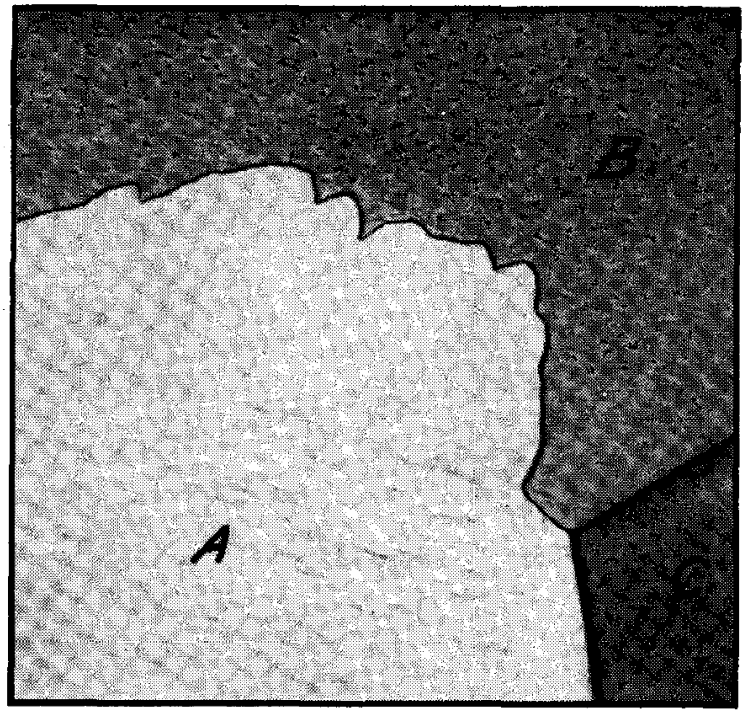
Participant Type: PD/PI
Participant: Moneesh Upmanyu
Person Months Worked: 9.00
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Funding Support:

Final Report:

This one-year project supported one graduate student and led to the following milestones:

A) **Impurity Effects on Morphological Stability of Recrystallization Fronts:** We investigates the origin of serrations during motion of recrystallization fronts. Past experiments have attributed the morphologies to the variations in the stored energy of deformation. The role of impurities has been ignored, although past studies have shown that front properties are dramatically altered by trace amounts of impurities. Here, we employ a combination of theoretical frameworks, Ising and molecular dynamics to study the influence of impurities on the stability of a moving recrystallization front, as determined by the balance between stored energy of deformation, solute drag and boundary stiffness. A linear stability analysis shows that the instability is enhanced at small impurity concentrations, and it is sensitive to the kinetics of impurities along and normal to the boundary. Our results underline the role of both driving forces and impurity diffusivities on the morphological stability of recrystallization fronts. In particular, the findings underscore the importance of solutes destabilizing recrystallization fronts in dilute alloys.



The findings were presented at a TMS Annual meeting, and will be followed by a peer-reviewed publication in this coming year.

B) Random Walk of a Solute Loaded fluctuating grain Boundary:

Tailoring the solute segregation at extended defects such as dislocations and interfaces is critical for engineering crystalline materials. Here, we use a combination of theoretical analyses and numerical simulations to study the effect of segregation on equilibrium fluctuations of grain boundaries. The random walk of the dirty interface occurs within a confining solute cloud that itself evolves stochastically in the crystalline matrix, albeit at a much slower rate. The coupled

response, a random walk within a random walk, represents a new class of stochastic dynamics. Numerical studies using a combination of Brownian dynamics, kinetic Ising model and all atom simulations of grain boundaries in Fe-C system reveal qualitatively different behavior at multiple time-scale. Our results have implications for direct quantification of solute effects on kinetics of grain boundaries, and more general interfaces. Interesting, the short-range fluctuations enable us to quantify the strength of interaction between the grain boundary and the solute, and therefore allow a rational design of stable nanocrystalline alloys. We are currently extending this study to polycystalline networks for a range of binary alloys.

C) Effect of solutes on grain boundary stiffness

The optimization of the grain size, morphology and topology is of critical importance during processing of nanocrystalline materials in order to enhance its optimum performance for variety applications. Grain boundary networks in nanocrystalline alloys are unstable due to the large curvatures that drive rapid coarsening. Adding solutes is an attractive strategy for suppressing coarsening as the kinetics of grain boundaries is considerably sensitive to solute content. In addition, solutes can also modify the grain boundary energy, and therefore their stiffness. The latter is a key quantity that dictates the coarsening kinetics, yet it has not been previously quantifies. In this work, we have employed capillarity fluctuation methods to explore interstitial solute effects on GB stiffness for an asymmetrical tilt grain boundary with different amounts of impurity concentration. Our results show that solute-loaded grain boundaries exhibit classical rough fluctuation spectrum that allows us to extract ther stiffness, and the stiffness increases non-linearly with the solute content. Our study offers a pathway for rational design of stable nanocrystalline alloys.